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# WW LCI v2: a second-generation life cycle inventory model for chemicals discharged to wastewater systems

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## Abstract

We present a second-generation wastewater treatment inventory model, WW LCI 2.0, which on many fronts represents considerable advances compared to its previous version WW LCI 1.0. WW LCI 2.0 is a novel and complete wastewater inventory model integrating WW LCI 1.0, i.e. a complete life cycle inventory, including infrastructure requirement, energy consumption and auxiliary materials applied for the treatment of wastewater and disposal of sludge and SewageLCI, i.e. fate modeling of chemicals released to the sewer. The model is expanded to account for different wastewater treatment levels, i.e. primary, secondary and tertiary treatment, independent treatment by septic tanks and also direct discharge to natural waters. Sludge disposal by means of composting is added as a new option. The model also includes a database containing statistics on wastewater treatment levels and sludge disposal patterns in 56 countries. The application of the new model is demonstrated using five chemicals assumed discharged to wastewater systems in four different countries. WW LCI 2.0 model results shows that chemicals such as diethylenetriamine penta (methylene phosphonic acid) (DTPMP) and Diclofenac, exhibit lower climate change (CC) and freshwater ecotoxicity (FET) burdens upon wastewater treatment compared to direct discharge in all country scenarios. Results for Ibuprofen and Acetaminophen (more readily degradable) show that the CC burden depends on the country-specific levels of wastewater treatment. Higher treatment levels lead to lower CC and FET burden compared to direct discharge. WW LCI 2.0 makes it possible to generate complete detailed life cycle inventories and fate analyses for chemicals released to

wastewater systems. Our test of the WW LCI 2.0 model with five chemicals illustrates how the model can provide substantially different outcomes, compared to conventional wastewater inventory models, making the inventory dependent upon the atomic composition of the molecules undergoing treatment as well as the country specific wastewater treatment levels.

**Keywords:** Environmental fate model; Life Cycle Inventory; Life cycle assessment; Sewage; Wastewater; WW LCI

## 1. Introduction

Wastewater is one of the main contributors to global environmental pollution. Whenever wastewater is emitted without adequate treatment, the untreated/partially treated wastewater pose various environmental impact potentials, such as marine and freshwater eutrophication and ecotoxicity. Although wastewater treatment can be the solution, treating wastewater is a resource-demanding activity, involving use of, among others, energy and chemicals. There are numerous approaches and technologies by which wastewater treatment can be achieved. However, to make wastewater treatment sustainable there is a need for more holistic/systemic assessments of wastewater treatment technologies. Life Cycle Assessment (LCA) has by now become a widely adopted approach for assessing environmental sustainability in the wastewater treatment sector (Corominas et al. 2013). A common foundation for including wastewater treatment in LCA studies is the Ecoinvent database, where inventories for wastewater treatment sourced in Switzerland are included. The Ecoinvent database uses the wastewater Life Cycle Inventory (LCI) model for Switzerland developed by (Doka 2007). These Ecoinvent inventories add uncertainty to the wastewater LCA given that the data on energy consumption, chemical consumption and infrastructures (wastewater and sewer) are specific for the location for which an inventory is generated, *i.e.* Switzerland in the Ecoinvent case, and yet they are used as representative inventories for many other countries in the world.

In addition, there is a growing content of trace pollutants in wastewater because of the ever increasing use of chemicals such as Pharmaceuticals and Personal Care Products (PPCP) (Muñoz et al. 2008; Jiang et al. 2013; Luo et al. 2014). A considerable fraction of such chemicals (pharmaceuticals, disinfectant etc.) are designed to have high biological activities are hence likely to cause effects in the environment upon emission. Complex organic molecules all behave

61 differently in wastewater treatment systems and pose different resource demands than more ordinary wastewater  
62 constituents such as inorganic chemicals (Muñoz et al. 2016). In order to correctly account for the environmental  
63 damages posed by these micro-pollutants upon emission to the environment even after wastewater treatment, there is a  
64 need for establishing dedicated life cycle inventories accounting for the resources needed to remove or more correctly  
65 lower the concentration of chemicals in wastewater upon treatment, as well as the particular fraction of the chemicals  
66 passing through the wastewater system and ending up in the environment via various elementary flows. The Ecoinvent  
67 model proves unsuitable to account for the diversity of chemical behavior in wastewater treatment systems since it  
68 assumes the same biodegradation coefficients (app. 53%) for all types of organic chemicals (Doka 2007, p. 18). Such  
69 simplification is inappropriate in the case of micro-pollutants such as e.g. PPCPs and for many other chemicals found in  
70 wastewater (Clark et al. 1995; Joss et al. 2006; Kujawa-Roeleveld and Schuman 2008). This highlights the need to  
71 develop dedicated inventories for assessing the environmental burdens associated with micro-pollutants emitted to  
72 wastewater systems.

73 Recently, there have been efforts in the direction of developing inventory models for micro-pollutants in wastewater.  
74 The model SewageLCI (Birkved and Dijkman 2012) was developed focusing on fate and transport of micro-pollutants  
75 in wastewater systems. The model provides the fraction of a chemical emitted to wastewater systems and subsequently  
76 undergoing fate processes in country/site specific steps of wastewater treatment (*i.e.* primary, secondary and tertiary  
77 treatment). A complete mass balance of the chemical being emitted to the wastewater system is provided as well as all  
78 the remaining fractions, such as the fraction emitted to air, surface water recipients and the fraction transferred to  
79 sludge. However, the SewageLCI model does not provide the complete inventory of the wastewater systems *i.e.* the  
80 inventory of the infrastructure required for wastewater treatment, energy consumption and other materials used during  
81 the treatment.

82 Muñoz et al. (2016) developed WW LCI 1.0, a model that provides the complete inventory of wastewater treatment  
83 systems. This model takes into account infrastructure requirements, energy consumption and auxiliary chemicals used  
84 for the treatment as well as sludge treatment including disposal hereof. The model also performs a mass balance of the  
85 chemicals emitted to the wastewater system. A limitation of this model is that it only considers wastewater treatment at  
86 secondary treatment level. Hence the model does not reflect the way in which the actual wastewater treatment systems  
87 are constructed and operated in most real-life situations. These past efforts suggest that although there have been  
88 attempts to provide inventory models for wastewater treatment for specific chemicals, none of these models are  
89 comprehensive, complete in nature and hence unable to properly provide real-life inventories.

In this paper, we present and demonstrate the WW LCI 2.0 model, which integrates the approach of SewageLCI (i.e. fate modeling of chemical released to the sewer), with the complete life cycle inventory (i.e. the inventory of infrastructure requirement, energy consumption and chemical used for the treatment of wastewater and disposal of sludge) approach of WW LCI 1.0. The developed integrated model addresses major limitations of past models, thus representing a substantial step forward. In addition, the model comes with a comprehensive country database on the wastewater treatment levels and practice of sludge handling applied in 56 countries.

## 2. Methodology

WW LCI 2.0 builds on the calculation modules of WW LCI 1.0. The reference flow for all the calculations remains unchanged *i.e.* “1 kg chemical discharged down the drain”. Table 1 shows the differences between the WWLCI 1.0 and WW LCI 2.0 model. As it can be seen from this table there are various new developments made in WW LCI 2.0 to improve the existing WW LCI 1.0 model. The new model presented here nevertheless differs from WW LCI 1.0 in the chosen approach for modelling of Wastewater Treatment Plants (WWTPs). Instead of considering only a standard WWTP with primary and secondary (biological) treatment, WW LCI 2.0 goes beyond this and further accounts for different levels of treatment. This approach of generating emissions inventory at treatment level was followed in Sewage LCI as reported in Birkved and Dijkman (2012). WW LCI 2.0 basically incorporates the features of WW LCI 1.0 and SewageLCI. Figure 1 shows the various components considered in the model and different percentages of wastewater along with the fractions of a chemical that are available as an output from the model. Figure 1 also shows that WW LCI 2.0 takes into account the direct discharge of wastewater to surface water and independent treatment in septic tanks, followed by disposal of septage.

In WW LCI 2.0, the input data requirement remains the same as in WW LCI 1.0, with only one additional chemical property required, namely the sludge-water partition coefficient ( $K_d$ ). Further, all calculations relating to biological treatment (organic matter removal, N removal), P removal, sludge digestion, energy use calculations and heat generation from sludge-derived biogas are the same as in the earlier version of the model.

Degradation of chemicals in the environment after the release to natural bodies was taken into account in WW LCI 1.0, according to the pathways described in Munoz et al. (2013). This approach of generating inventories for chemicals (i.e. with inclusion of environmental degradation) is retained in WW LCI 2.0. However, as degradation takes place in the ecosphere, and should be captured in impact assessment calculations rather than in the inventory analysis (Muñoz et al.

2013), in WW LCI 2.0 an additional option of creating inventory without accounting for environmental degradation is provided. Users can choose this inventory generation option according to the system boundary preferences.

The following sub-sections describe in detail the new features of WW LCI 2.0, namely the underlying data sources, calculations and assumptions.

## 2.1 WWTP with Primary treatment only

WWTPs applying only primary treatment have been modelled as a conventional sedimentation tank. The main purpose of primary treatment is to remove suspended solids. Primary treatment typically achieves 30% Biochemical Oxygen Demand (BOD) removal efficiency and 30% removal of Suspended Solids (SS) in primary sludge (Metcalf et al. 2007). Using the same approach, the degradation and sorption to sludge rates for a given chemical are calculated in accordance with Eqs. 1 and 2:

$$F_{deg.pt} = r_{deg.pt} \times F_{deg.as} \quad (1)$$

$$F_{sludge.pt} = r_{sludge.pt} \times F_{sludge.as} \quad (2)$$

Where,  $F_{deg.pt}$  is the fraction of chemical biodegradation in WWTPs with primary treatment only,  $F_{deg.as}$  is the fraction of biodegradation in full-fledged WWTPs (primary treatment followed by activated sludge process),  $r_{deg.pt}$  is the ration (expressed in percentage) of degradation efficiency in WWTPs with only primary treatment to degradation efficiency in full scale WWTPs (typically considered as 30%).

$F_{sludge.pt}$  is the fraction of solids removal in WWTPs with primary treatment only,  $F_{sludge.as}$  is the fraction of solids removed in full-fledged WWTPs,  $r_{sludge.pt}$  is the ration (expressed in percentage) of SS removal efficiency in WWTPs with only primary treatment to SS removal efficiency in full scale WWTP (typically considered as 30%).

In this way, removal rates of a given chemical in a WWTP with only primary treatment are thus linked to the rates of full-fledged WWTP applying primary and secondary treatment, which are available from the data introduced by the user. This has the advantage that additional input data in terms of removal rates for primary treatment are not required, thus reducing the data collection burden for the user.

Infrastructure requirements for primary treatment are considered as 30% of an entire WWTP (including all tanks, buildings, anaerobic digester, etc.) in accordance with the inventory processes available in the Ecoinvent 3.2 database.

143 This infrastructure demand is a rough estimate and it is based on the assumption that infrastructure demands are  
 144 proportional to the overall area requirements of a WWTP. A plant applying only primary treatment requires roughly  
 145 70% less area than a complete WWTP, given that elements such as biological reactors, settling tanks, and anaerobic  
 146 digesters are not needed. These assumptions are incorporated as parameters in the model and the user can change the  
 147 default parameter values if better data should become available. The electricity requirement for primary treatment were  
 148 interpolated from the detailed energy consumption reported for US WWTPs by (Stillwell 2010). All the parameters and  
 149 data related to primary treatment are provided in the Supplementary Information (SI) in Table S1.

## 150 **2.2 Tertiary treatment**

151 Small particles of sludge which are not settled in secondary settling tank pass on to the next level of treatment or get  
 152 discharged with secondary treated wastewater. The fraction of a chemical sorbed to these particles is hence emitted  
 153 along with these sludge particles, which can be removed by filtration. Sand filtration is considered as the only tertiary  
 154 treatment in WW LCI 2.0. The inventory for energy requirements and infrastructure requirements of sand filtration was  
 155 derived from (Muñoz et al. 2010). All parameters and data related to tertiary treatment are provided in the SI in Table  
 156 S1. The fraction of the chemical adsorbed to the suspended solid phase in the effluent reaching the sand filter can be  
 157 estimated according to Stuer-Lauridsen et al. (2000):

$$158 \quad K_d = f_{oc} \times 0.41 \times K_{ow} \quad (3)$$

159 *Where:*

160  $sK_d$  is the sludge-water partition coefficients [-]

161  $f_{oc}$  is the fraction of organic carbon in sludge [-]

162  $K_{ow}$ , is the octanol-water distribution coefficient of the compound I [-]

163 In case of dissociating compounds (in this case acids and bases according to the Brønsted–Lowry acid–base definition)

164  $D_{ow}$  should be used instead of  $K_{ow}$  and eq. 3 can be reformulated as:

$$165 \quad K_d = f_{oc} \times 0.41 \times D_{ow} \quad (4)$$

166 *Where:*

$D_{ow}$  is the pH corrected octanol-water distribution coefficient of an organic chemical compound accounting for the pH dependency of  $K_{ow}$  induced by the presence of ionisable groups in an organic molecule [-]

$D_{ow}$  can be estimated as:

$$D_{ow} = \frac{K_{ow}}{1 + 10^{(pH - pK_a)}} \quad (5)$$

Where:

$pH$  is the pH of the effluent of tertiary treatment [-]

$pK_a$ , is the acid dissociation constant of chemical compound [-]

Depending on the chemical properties, the fraction of a chemical sorbed to the sludge can be based on either  $K_d$  or  $D_{ow}$  using the following equation (Andersen et al. 2004):

$$F_{sludge,tt} = \frac{\rho_{sludge} \times K_d}{1 + \rho_{sludge} \times K_d} \quad (6)$$

Where:

$\rho_{sludge}$  is the density (dry solid) of the sludge [g/L]

### 2.3 Septic tank

Septic tanks are still a common treatment choice in emerging economies (Tilley et al. 2008). Septic tanks are known to remove 30% BOD and achieve 30% removal of SS (Mara 1996; Crites and Technobanoglous 1998). Following an approach similar to the one used for WWTPs having only primary treatment, we estimate the chemical-specific degradation and sludge sorption rates by interpolating from the corresponding rates for a WWTP applying primary and secondary treatment, as in Eqs. 7 and 8:

$$F_{deg,st} = r_{deg,st} \times F_{deg,as} \quad (7)$$

$$F_{sludge,st} = r_{sludge,st} \times F_{sludge,as} \quad (8)$$

Where,  $F_{deg,st}$  is the fraction of chemical removed by biodegradation in septic tanks

$F_{deg,as}$  is the chemical specific fraction of biodegradation in a full-fledged WWTP



$r_{deg.st}$  is the ratio (expressed in percentage) of degradation efficiency in septic tank relative to degradation efficiency in full-fledged WWTP (typically as assumed to be 30%).

$F_{sludge.st}$  is the fraction of solids removed in a septic tank

$F_{sludge.as}$  is the fraction of solids removed in a full-fledged WWTP

$r_{sludge.st}$  is the ration (expressed in percentage) of SS removal efficiency in septic tank to SS removal efficiency in full scale WWTP (typically considered as 30%).

The data related to infrastructure requirements for septic tanks were obtained from Pizzol et al. (2015). All parameters and data related with the septic tank submodel are provided in SI in Table S1. Sludge stored in septic tanks is considered to undergo spontaneous anaerobic digestion before extracted for disposal. In our model this anaerobic digestion is modelled as in WW LCI 1.0 (Muñoz et al. 2016), however biogas generated from this chemical reaction is not collected and escapes to the atmosphere. The septage (the sludge extracted from septic tanks) is assumed to be transferred by a truck and transported (50 km) to a WWTP, where it joins the sludge line. No further chemical transformations are taken into account for the septage once it enters the WWTP, and only energy and infrastructure requirements associated with sludge handling in the WWTP are taken into account.

## 2.4 Sludge composting

Sludge composting is modeled based on a windrow composting process. The compost plant infrastructure is based on the Ecoinvent data set for a compost plant treating 10,000 ton waste in wet weight per year, with a service life of 25 years (Nemecek and Kägi 2007). Electricity and diesel use for a sludge composting plant operation was obtained from (Poulsen and Hansen 2003). The conversion of sludge into compost is based on a mass balance, where only degradable elements in sludge are affected by the composting process. We use the same definition of degradable/inert organic matter as in Muñoz et al. (2016). Dry mass reduction for degradable organic matter is assumed to be 65%. This reduction represents the arithmetic average reduction reported for five fractions commonly found in putrescible organic matter (lignin, cellulose, carbohydrate, fat, protein) in (Sonesson 1996). Emissions produced by the composting process include CO<sub>2</sub>, methane, N<sub>2</sub>O, N<sub>2</sub>, ammonia and NO<sub>x</sub>. Methane emissions are calculated as 0.01 kg CH<sub>4</sub>/kg degradable organic matter in dry mass (IPCC 2006), assuming that typical organic matter (food and garden waste) contains 0.435 kg carbon/kg dry mass (IPCC 2006). Nitrogen in degradable organic matter is emitted as 2% N-N<sub>2</sub>O, 2% N<sub>2</sub>, 96% N-NH<sub>3</sub> based on (Sonesson 1996). In addition, we take into account that 15% of the emitted ammonia is converted to NO<sub>x</sub> as a secondary pollutant (FAO and IFA 2001). Thus, the 96% N-NH<sub>3</sub> is in fact modeled as 82% N-NH<sub>3</sub> and 14% N-

217 NO<sub>x</sub>. Based on typical values for moisture content in input sludge (Poulsen and Hansen 2003), wet mass reduction  
218 during composting (Poulsen and Hansen 2003) as well as moisture content in compost (Sonesson 1996), a fixed water  
219 evaporation rate of 70% of the water input is obtained. For mass balance purposes, the consumption of atmospheric  
220 oxygen during composting is calculated, based on the stoichiometric requirements to form CO<sub>2</sub> from carbon in  
221 degradable organic matter. The amount of final compost obtained in wet weight is calculated with Eq. 9:

$$\text{Compost} = (\text{sludge input} + \text{O}_2) - (\text{water evaporation} + \text{CO}_2 + \text{CH}_4 + \text{N}_2 + \text{N}_2\text{O} + \text{NH}_3 + \text{NO}_x) \quad (9)$$

223 Based on the initial composition of sludge entering the composting plant and the detailed mass balance, the composition  
224 of the resulting compost is obtained, including the fraction (if any) of original chemical released down the drain still  
225 remaining in the compost. This composition is used as input for the calculations dealing with application of compost in  
226 agriculture, which follows the same principles as sludge application in agriculture in accordance with WW LCI 1.0  
227 (Muñoz et al. 2016).

## 228 **2.5 Country database**

229 WW LCI 2.0 provides a database on the current status of wastewater treatment levels and sludge disposal practices in  
230 56 countries, based on a wide variety of public sources such as Eurostat, OECD statistics as well as country-specific  
231 statistics. Data for 56 countries, on population fractions connected to urban wastewater collection systems - without  
232 treatment (%), with primary treatment (%), with secondary treatment (%) and with tertiary treatment (%) are included.  
233 Also, population fractions connected to independent wastewater collecting systems with treatment (%) and without  
234 treatment is available in the database. For sludge management the percentage of sludge being sent for agriculture,  
235 composting, incineration or landfill is also available for all the 56 countries. These statistics are automatically loaded as  
236 input data to the model, thus providing a basis for country-specific LCIs. Nevertheless, an option is provided for the  
237 user to override these default data in case more accurate data should become available.

## 238 **2.6 Application to five chemicals**

239 In order to show its applicability in practice, we have assessed five chemicals with WW LCI 2.0. Four chemicals  
240 (Ibuprofen, Acetaminophen, DTPMP and Diclofenac) are commonly used in PPCPs and the fifth chemical is Atrazine,  
241 which is commonly used as herbicide. The occurrence of these five chemicals in trace amounts is common in sewage  
242 (Muñoz et al. 2008; Jiang et al. 2013; Luo et al. 2014). Table 2 shows the list of chemicals with their key features.  
243 These molecules have different chemical compositions, biodegradability and toxicities. To further demonstrate the

244 usefulness of the tool, these five chemicals are assessed in four countries *viz.* Denmark (DK), United States of America  
245 (US), China (CN) and India (IN). This choice of countries allows us to model and assess differences in terms of  
246 developed vs. developing countries, as well as differences in levels of wastewater treatment and sludge disposal  
247 practices (Table 3).

248 Table S2 in the SI shows the physico-chemical properties of these five chemicals. These physico-chemical properties  
249 were used to determine fate in the WWTP by using steady-state WWTP simulation models. Various steady-state and  
250 dynamic models are available for modelling WWTPs (Gujer et al., 1999; Grau et al., 2007; Ekma, 2009). We have used  
251 SimpleTreat (Franco et al. 2013a; Franco et al. 2013b), the model implemented in the European Union framework for  
252 the environmental risk assessment of chemicals, to obtain fate factors of these chemicals in a WWTP applying primary  
253 treatment plus biological treatment by means of activated sludge. USES-LCA (Van Zelm et al. 2009), which is included  
254 in WW LCI 2.0, is used to estimate the fate of the chemicals in the environment (when emitted to either air, water or  
255 soil). These fate factors are provided in Table S3 in SI.

256 Life Cycle Impact Assessment (LCIA) at mid-point level was carried out by importing the inventories generated by  
257 WW LCI 2.0 to Simapro 8.0.4. Four relevant impacts categories were assessed using Simapro 8.0.4. The climate change  
258 impact category was assessed by means of the global warming potential (GWP) considering a time horizon of 100 years  
259 (Forster et al. 2007). Eutrophication (freshwater and marine) impacts were assessed using ReCiPe method (Goedkoop et  
260 al. 2008) and USEtox v2.0 (Rosenbaum et al. 2008) was used to assess Freshwater Ecotoxicity (FET) impacts.  
261 Terrestrial ecotoxicity was not included in the assessment since USEtox does not currently cover this impact category.

## 262 **3. Results and discussion**

### 263 **3.1 Inventory results**

264 Key foreground inventory results obtained from WW LCI 2.0 for the five chemicals assessed in four countries are  
265 presented in Table S4 in SI. The inventory results reveal that different chemicals involve different resource (energy and  
266 chemicals) consumption in each of the four country scenarios.

267 In DK and US Diclofenac and DTPMP show a net negative electricity consumption, meaning that treatment of these  
268 chemicals produces more energy than what additionally is required by the WWTPs and sludge disposal. This is caused  
269 by a relatively high sludge production from treatment of effluents containing these two chemicals combined with the  
270 fact that the sludge is combustible, achieving credits from energy recovery in relation to sludge incineration. Presence

271 of the remaining three chemicals induces demand for more electricity than can be produced using sludge incineration in  
272 the 4 countries. In China and India lower (i.e. lower than in DK and US) wastewater treatment levels prevails (both in  
273 terms of secondary as well as tertiary treatment, see Table 3) entailing lower sludge productions from WWTPs in China  
274 and India. This leads to a net demand for electricity (*i.e.* credits from sludge digestion since sludge incineration does not  
275 compensate for the electricity requirement for treatment and sludge disposal). Overall, a chemical that is easily  
276 biodegradable (e.g. Ibuprofen), has a higher electricity demand compared to a chemical which is non-biodegradable  
277 since it undergoes biological treatment and hence consumes more electricity for e.g. aeration in a WWTP with  
278 secondary treatment.

279 For the treatment of wastewater in cold climate countries such as Denmark there is a heat requirement for maintaining  
280 optimal temperatures in the aeration tank. This requirement induces the heat consumption, which can be supplied using  
281 co-generation of heat and electricity through sludge incineration. The net balance between the heat required by the  
282 treatment process and heat produced using co-generation defines whether there will be positive consumption of the heat  
283 or there will be surplus heat generates. Net heat consumption for all chemicals in all countries is found to be negative  
284 except for DTPMP in China and India (see Table S4). The reason remains the same as explained for electricity, i.e. the  
285 heat produced from sludge digestion and incineration does not compensate for the heat required to operate the WWTP  
286 and sludge digestion in CN and IN. This is because the sludge generated by the biodegradable chemicals (e.g. Ibuprofen  
287 and Acetaminophen) consists of biomass with a high moisture content (intracellular water) which is not removed by  
288 dewatering, whereas non-degradable chemicals such as DTPMP do not yield higher moisture levels of the sludge. Non-  
289 degradable organic chemicals do not result in an increased presence of biomass in the sludge but rather in an increased  
290 carbon content of the sludge.

291 Sludge production is relatively high (0.3 to 0.8 kg dry mass/kg chemical) for chemicals that exhibit partition preference  
292 towards the solid phase, such as Diclofenac and DTPMP. For Diclofenac this relates to the presence of tertiary  
293 treatment in DK and US, while for DTPMP tertiary treatment is not required to cause partitioning to sludge. Chemicals  
294 that are at the same time non-biodegradable and do not tend to partition to the solid phase (*e.g.* Atrazine) yield lower  
295 sludge productions (0.02 kg dry mass/kg chemical).

296 Wastewater treatment also leads to credits originating from avoided mineral fertilizers in those cases where sludge  
297 generated in WWTPs is applied to agricultural land. The amount of substituted fertilizer depends on the N and P content  
298 of the chemicals undergoing treatment, the chemical's biodegradability and water-sludge partitioning, the country

specific level of wastewater treatment and sludge management practices (i.e. use in agriculture). As it can be seen from Table S4, DTPMP obtains relatively high credits for avoided phosphate fertilizer (about -0.2 kg P<sub>2</sub>O<sub>5</sub>/kg chemical in Denmark and US and -0.16 kg P<sub>2</sub>O<sub>5</sub>/kg chemical in India). In China, only 33% of the wastewater undergoes treatment and only about 50% of the sludge produced in WWTPs is applied to arable land, the fertilizer credit obtained by DTPMP is low (-0.09 kg P<sub>2</sub>O<sub>5</sub>/kg chemical). For the remaining chemicals, which do not have P in the molecule still lower nutrient credits are achieved due to nitrogen content in sludge.

Direct CO<sub>2</sub> emissions from the discharge of these chemicals can be grouped into four categories *viz.*, emissions from the WWTP (process emissions due to biodegradation), emissions from sludge disposal, degradation of the chemicals in the environment and long-term storage (*e.g.* landfill). Emissions from the WWTP are higher for Ibuprofen and Acetaminophen in Denmark and US given that in these countries the population fractions connected to WWTPs are high and because these chemicals undergo degradation during biological treatment. Chemicals partitioning to the solid phase end up in the sludge and therefore exhibit significant CO<sub>2</sub> emissions in relation to sludge disposal (*e.g.* Diclofenac). In China and India, most of the CO<sub>2</sub> emissions are associated with degradation of chemicals in the environment, as there is a relatively low fraction of the populations connected to wastewater treatment in these countries.

One of the more interesting features of WW LCI 2.0 is that the user can obtain a complete impact assessment profile for the chemical released down the drain. The last three rows in Table S4 show, for each of the 5 chemicals, the respective fractions emitted to air, water and soil. More persistent chemicals that tend to partition to sludge such as DTPMP and Diclofenac appear as emissions to soil in the inventory for those countries where sludge is used in agriculture. Persistent chemicals that do not undergo considerable degradation within a WWTP, such as Atrazine, are mainly released to surface water. Surface water is obviously also the main environmental compartment of emission for all chemicals in China and India, where connection to WWTPs by the population is low. Hence, a further impact assessment of such emissions needs to be carried out to determine the health and ecosystem damages due to emission of these chemicals to ambient water.

### 3.2 Life cycle impact assessment

Figure 2 shows the impact assessment results for climate change (CC) for all five chemicals in each country. A direct discharge scenario (0% connection to any type of wastewater treatment) is for comparative purposes shown as reference.

327 DTPMP shows a value of 1.7 kg CO<sub>2</sub> eq. /kg released when wastewater is discharged directly without any treatment.  
 328 Compared to this value, DK and US show CC values of 0.6 and 0.7 kg CO<sub>2</sub> eq. /kg released. These lower values can be  
 329 explained by the fertilizer credit achieved by DTPMP in these countries as well as to the fact that in the direct discharge  
 330 scenario DTPMP degradation is expected to form some methane (Munoz et al., 2016), which is avoided if the chemical  
 331 passes through WWTPs. In China and India DTPMP cause emissions of 1.2 and 1.5 kg CO<sub>2</sub> eq. /kg released. The higher  
 332 value obtained for India is due to the lower fertilizer credits and higher impact of electricity production used for aeration  
 333 in WWTPs. The results for the remaining three chemicals (Ibuprofen, Diclofenac and Acetaminophen) can be explained  
 334 in a similar way. Overall, DK and US exhibit lower CC impact potentials for treatment compared to direct discharge  
 335 scenarios due to higher levels of secondary and tertiary treatment (and hence higher electricity credits from sludge  
 336 incineration, see Table S4 in SI). In China and India the lower treatment levels, together with a considerable  
 337 environmental impacts induced by electricity production due to substantial use of fossil fuels causes the CC impact  
 338 potentials of the treatment scenarios to equal those for direct discharge. For Atrazine, which is removed neither by  
 339 secondary nor tertiary treatment, the CC impact potentials in all four countries are almost equal (in DK and CN) or  
 340 higher (in US and IN) compared to direct discharge scenarios. The reason for this is that there is no removal of Atrazine  
 341 at any stage of the wastewater treatment, and only little additional impact is induced by infrastructure and energy  
 342 requirements in the WWTP.

343 The FET indicator results exhibit a pattern somewhat similar to the CC impact potential as the FET results show similar  
 344 ranking of the chemicals in each country-specific scenario, except Atrazine (refer to Figure 3). Overall, Denmark and  
 345 US obtain lower FET impact potentials compared to China and India for DTPMP, Ibuprofen, Diclofenac and  
 346 Acetaminophen. Due to its high ecotoxicological impact potential according to USEtox, Atrazine exhibits high FET  
 347 impact potentials in all the scenarios. For all five chemicals, it is observed that FET results for the direct discharge  
 348 scenarios are higher than in any of the country specific scenarios including treatment. As expected, wastewater  
 349 treatment mitigates freshwater ecotoxicity impacts, as long as chemicals are effectively removed by the treatment. The  
 350 toxicity impact potentials induced by the WWTP's background system (electricity production, infrastructure  
 351 production, etc.) are lower than the toxicity impacts induced by these chemicals irrespective of wastewater treatment.

352 The freshwater eutrophication impact potentials (FEP) and the marine eutrophication impact potentials (MEP) are  
 353 presented in Figure 4. Chemicals having Nitrogen (N) and/or Phosphorus (P) in their chemical structure exhibit  
 354 substantially higher FEPs and MEPs. As DTPMP contains 5 atoms of P per molecule and Atrazine contains 5 atoms of  
 355 N per molecule, DTPMP and Atrazine yields higher values for FEP and MEP, respectively. Atrazine, Diclofenac and

356 Acetaminophen yields lower FEP compared to DTPMP as these chemicals do not contain P atoms. For all these  
357 chemicals, the contribution to FEP originates from the background system (production of energy, auxiliary materials,  
358 etc.). It should be highlighted that even though Ibuprofen does not contain N or P, some small contributions for FEPs  
359 and MEPs are observed in Figure 4. These impacts are caused by N in the sludge biomass generated during the  
360 biological treatment in the WWTP.

### 361 **3.3 Uncertainties and Limitations of the model**

362 Although the present model goes beyond WW LCI 1.0, it still shares many of its inherent limitations, as discussed by  
363 Muñoz et al. (2016). Below we list what in our opinion are the main limitations of WW LCI 2.0:

- 364 i. The country database on wastewater treatment levels and sludge management practices was derived from  
365 various literature sources. These data have a strong influence on the LCIs produced by the model. Although  
366 the values reported in the database can be considered as reasonable, the user needs to assess the quality of  
367 these data and decide whether or not other more reliable data sources are available.
- 368 ii. Removal efficiencies of organic matter and suspended solids in septic tanks and primary sedimentation tanks  
369 are estimated based on literature. These removal efficiencies are then made chemical-specific based on the  
370 values for the same chemical in a WWTP using activated sludge. This approach was chosen to minimize the  
371 data collection efforts, which for the present version of our model is substantial, but on the other hand  
372 constitutes a simple way of modeling the treatment process.
- 373 iii. Tertiary treatment is limited to pressure sand filtration. This is a simplification of reality, since there is  
374 currently a wide range of tertiary or advanced treatment methods, such as membrane filtration (from  
375 microfiltration to reverse osmosis), disinfection, or advanced oxidation processes (ozonation, photocatalysis).  
376 These technologies are not considered in the model.
- 377 iv. Application of wastewater, either treated or untreated, for irrigation of crops or for other uses is not currently  
378 included and therefore the model neither accounts for the potential environmental benefits in terms of  
379 freshwater resource conservation, nor for the potential impact on terrestrial ecotoxicity derived from  
380 chemicals deposited in soil through this emission pathway.
- 381 v. As opposed to SewageLCI, WW LCI 2.0 does not consider degradation of chemicals in the sewer before they  
382 reach the WWTP.

- vi. Management of septage (sludge from septic tanks) is assumed to be treatment in a WWTP. Although this might seem appropriate in the context of a developed country, in developing countries this assumption could be far from reality, given that there are many options currently applied to deal with such waste, from dedicated septage treatment plants to simple discharge of the septage into open drains.
- vii. As in WW LCI 1.0, electricity mixes are country-specific, thus allowing for differentiation of impacts induced by different national electricity mixes. On the other hand, thermal energy production is by default assumed based on natural gas, which may not be realistic in countries like e.g. China, where the use of coal is prevailing.
- viii. In relation to secondary treatment in WWTPs those chemicals that do not contain N in their molecule are assumed to benefit from ‘free’ N (e.g.  $\text{N-NH}_4^+$ ) available in wastewater, in order to form sludge biomass. However, as a consequence of this N consumption, the treatment of this amount of N by the WWTP (through nitrification and denitrification) is avoided, however this trade-off is not accounted for by the model. This limitation was inherent to WW LCI 1.0 (although not discussed by the authors) and still present in the new version. In this way, the environmental impact of chemicals that do not contain N in their molecule is (slightly) overestimated.

Despite of the above listed uncertainties and limitations related with the model, the WW LCI 2.0 model represents an advancement in the area of wastewater treatment inventories. The model is as far as we know an important applicable missing link between chemical consumption and chemical emission in LCA, especially for chemicals present in products with wide-dispersive use patterns such as e.g. PPCPs.

## 5. Conclusions

In this paper we have presented WW LCI 2.0, a second-generation model resulting from the integration of two existing models, namely SewageLCI 1.0 and WW LCI 1.0. The purpose of this model is to provide LCIs for specific chemicals under average treatment practices in different countries, and not the assessment of wastewater treatment technologies. The new integrated model generates chemical-specific LCIs of chemicals released to the sewer systems, according to country-specific conditions in terms of wastewater treatment levels as well as typical sludge disposal practices. The resulting inventories take into account the mass balance of the chemical undergoing treatment and all the required



411 inputs from technosphere (energy, chemicals, infrastructure, *etc.*). The applicability of this model has been  
412 demonstrated by applying it to five chemicals commonly occurring at trace levels in wastewater.  
413 Each of the five chemicals assessed yielded quite different inventories and hence different impact profiles owing to the  
414 fact that different chemicals will have different level of wastewater treatment demands. The major findings of our work  
415 are:

- 416 i. Similar chemicals yield different inventories in the country specific scenarios, and it has hence been illustrated  
417 that different treatment strategies and trade-off options will yield different inventories also for similar  
418 chemicals.
- 419 ii. The energy required for wastewater treatment of biodegradable chemicals can be compensated for by the  
420 electricity produced from sludge incineration.
- 421 iii. For highly persistent chemicals like Atrazine, indirect toxicity related impacts from treatment systems  
422 (including electricity production, production of chemicals, infrastructure, *etc.*) are lower than direct toxicity  
423 related impacts, exerted by these chemicals, when emitted to the environment after treatment.
- 424 iv. Treatment of wastewater is recommended up to the tertiary level in order to reduce environmental impacts  
425 such as eco-toxicity and eutrophication, but also climate change.
- 426 v. The model also proves the relevance of sludge disposal practices in terms of the environmental impact trade-  
427 offs.

428 In spite of its limitations, WW LCI 2.0 constitutes a considerable step forward in the modelling of life cycle inventories  
429 for chemicals, allowing LCA practitioners to get a more realistic picture of how chemicals contribute to the  
430 environmental impacts caused by wastewater discharges.

431

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512

513

514 Table 1: New developments in WW LCI 2.0 and major differences with WW LCI 1.0

			WW LCI v1	WW LCI v2
Wastewater treatment levels	WWTP with primary treatment only		✗	✓
	WWTP with primary & secondary treatment	With N removal	✓	✓
		Without N removal	✓	✓
	As above, plus tertiary treatment (sand filter)		✗	✓
	Chemical phosphorus removal		✓	✓
	Septic tanks		✗	✓
	No treatment (direct discharge)		✓	✓
Sludge disposal	Composting		✗	✓
	Landfarming		✓	✓
	Landfilling		✓	✓
	Incineration		✓	✓
Database	Wastewater treatment statistics		✗	✓
	Sludge disposal statistics		✗	✓
LCI results	Exportable to SimaPro		✓	✓
	Possibility of excluding environmental degradation emissions		✗	✓

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517

518 Table 2. Key features of the five chemicals assessed

Name	CAS number	Key features
Diclofenac	15307-86-5	Organic, poorly degradable, contains N and fossil C*
Ibuprofen	15687-27-1	Organic, degradable, contains fossil C*
Atrazine	1912-24-9	Organic, poorly degradable, contains N, contains fossil C*
Diethylenetriamine penta (methylene phosphonic acid) (DTPMP)	15827-60-8	Organic, soluble, contain N and P, contains fossil C*
Acetaminophen	103-90-2	Organic, degradable, contains N, contains fossil C*

519 \* Assumed for the purpose of the study.

Table 3: National wastewater treatment levels and sludge handling practice at four countries assessed

		DK	US	CN	IN
Wastewater treatment scenario	Connection to urban wastewater collecting systems - total (%)	89%	81%	46%	21%
	Connection to urban wastewater collecting systems - without treatment (%)	0%	6%	13%	0%
	Connection to urban wastewater collecting systems - with treatment (%)	89%	76%	33%	21%
	Connection to urban wastewater treatment - primary treatment (%)	2%	6%	0%	0%
	Connection to urban wastewater treatment - secondary treatment (%)	3%	29%	33%	21%
	Connection to urban wastewater treatment - tertiary treatment (%)	84%	41%	0%	0%
	Connection to independent wastewater collecting systems - total (%)	11%	19%	54%	79%
	Connection to independent wastewater collecting systems - with treatment (%)	11%	19%	0%	39%
	Connection to independent wastewater collecting systems - without treatment (%)	0%	0%	54%	39%
Sludge scenario	Sludge to composting (%)	6%	12%	4%	0%
	Sludge to landfarming (%)	50%	41%	52%	100%
	Sludge to landfilling (%)	0%	32%	40%	0%
	Sludge to incineration (%)	44%	16%	4%	0%

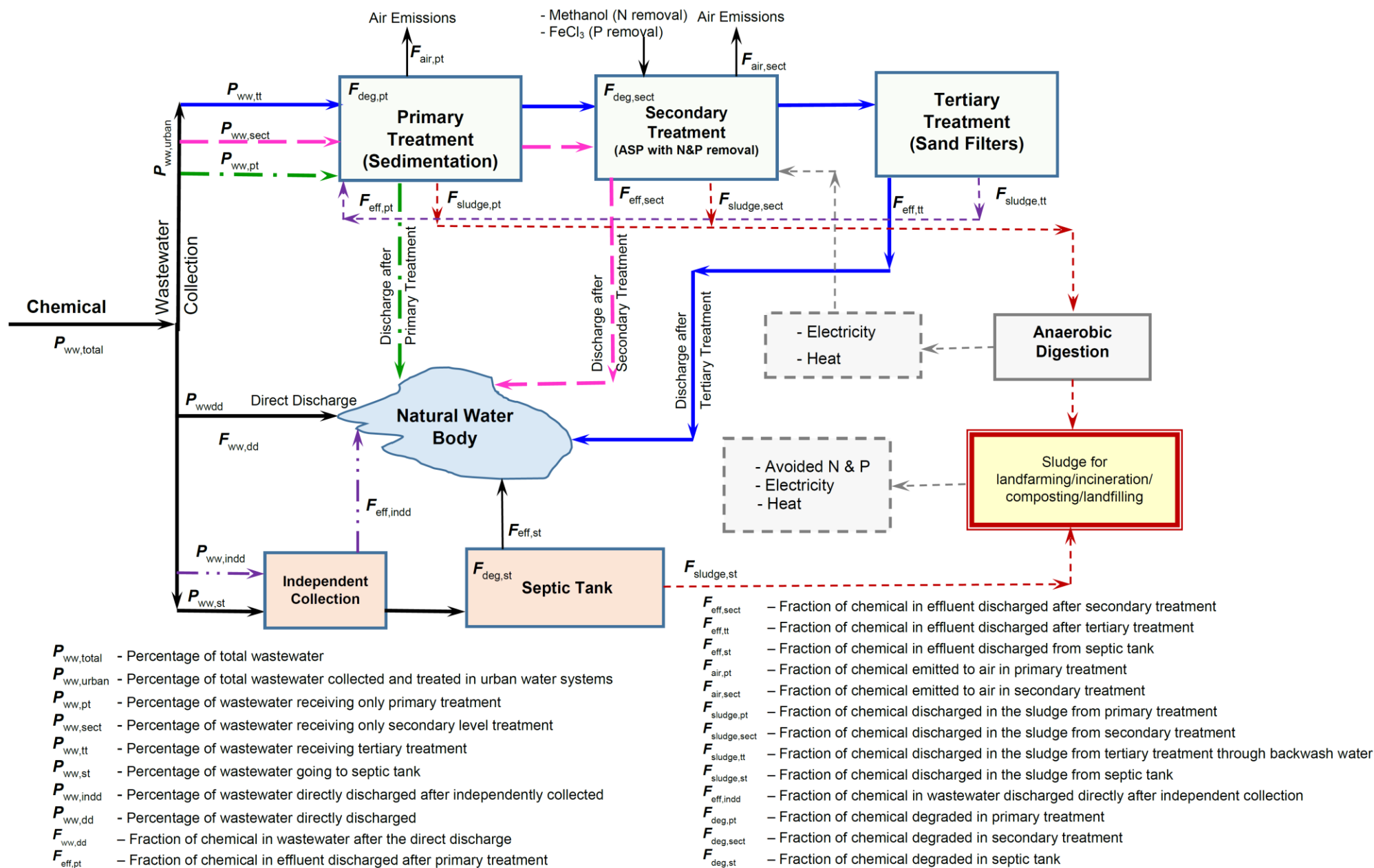


Figure 1: Flow scheme for WW LCI 2.0



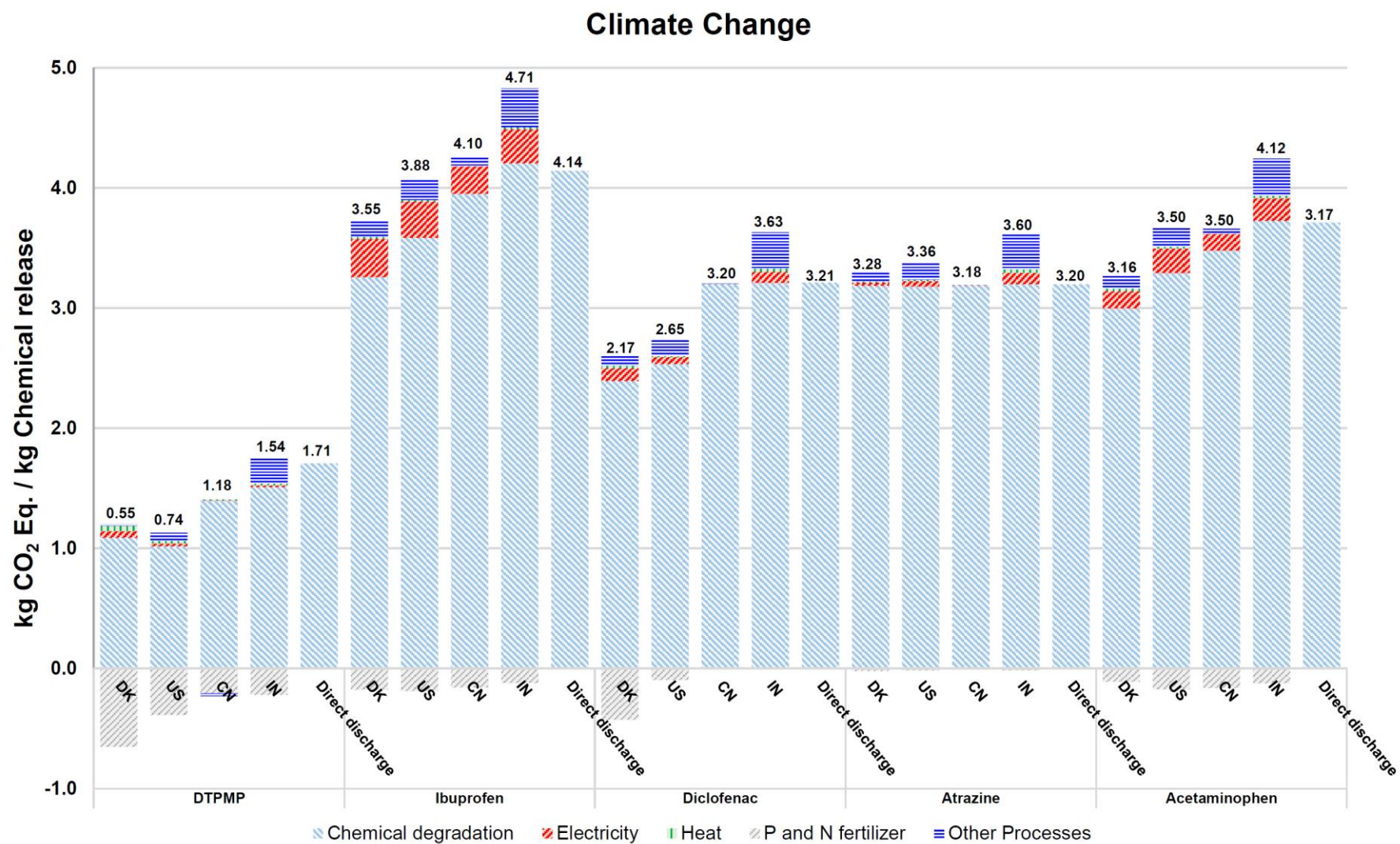


Figure 2: Impact assessment results for climate change indicator (values on the top of columns represents net climate change value i.e. after deducting credits)

## Freshwater Ecotoxicity

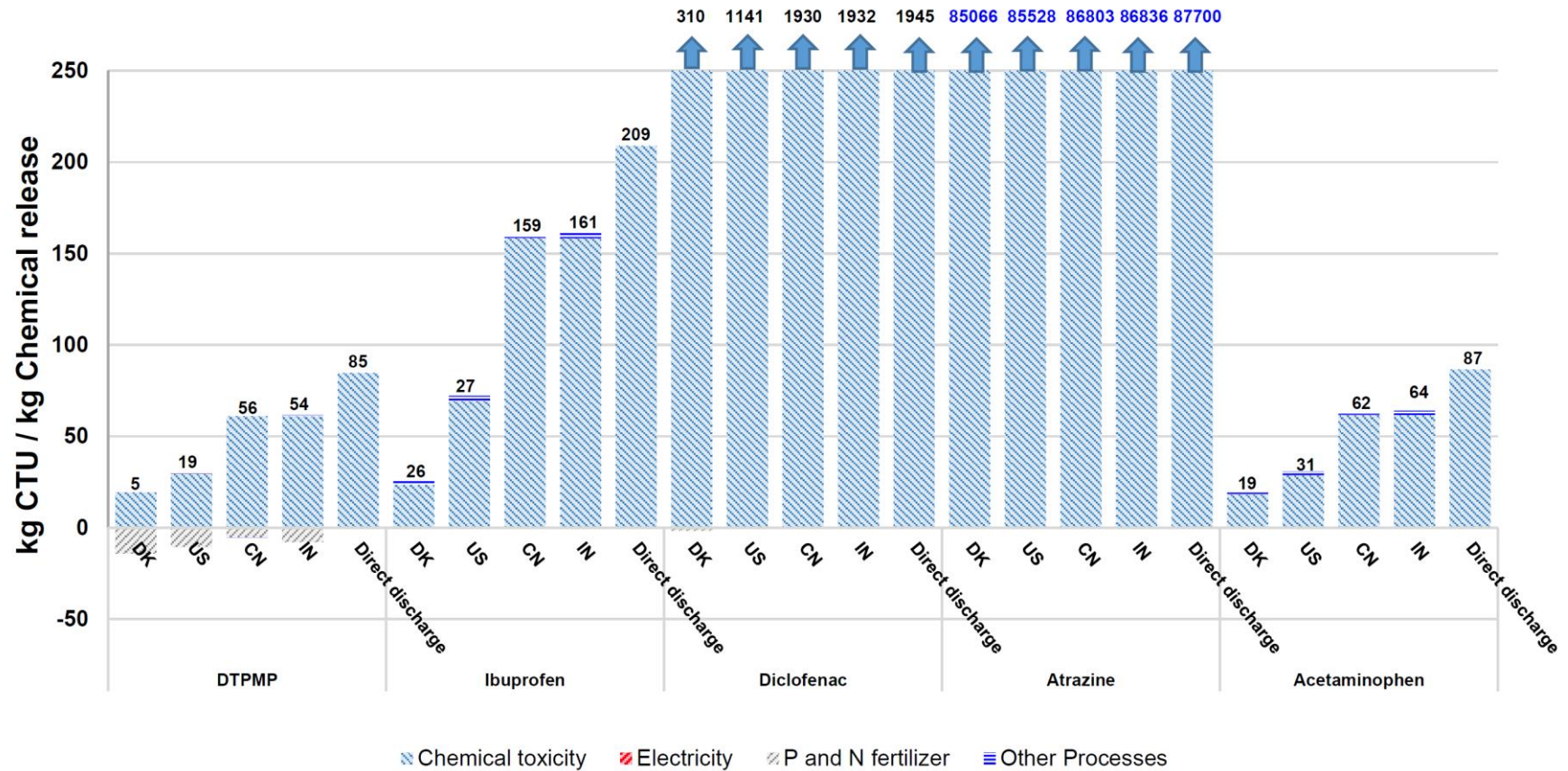


Figure 3: Impact assessment results for freshwater ecotoxicity (values on the top of columns represents net climate change value i.e. after deducting credits)

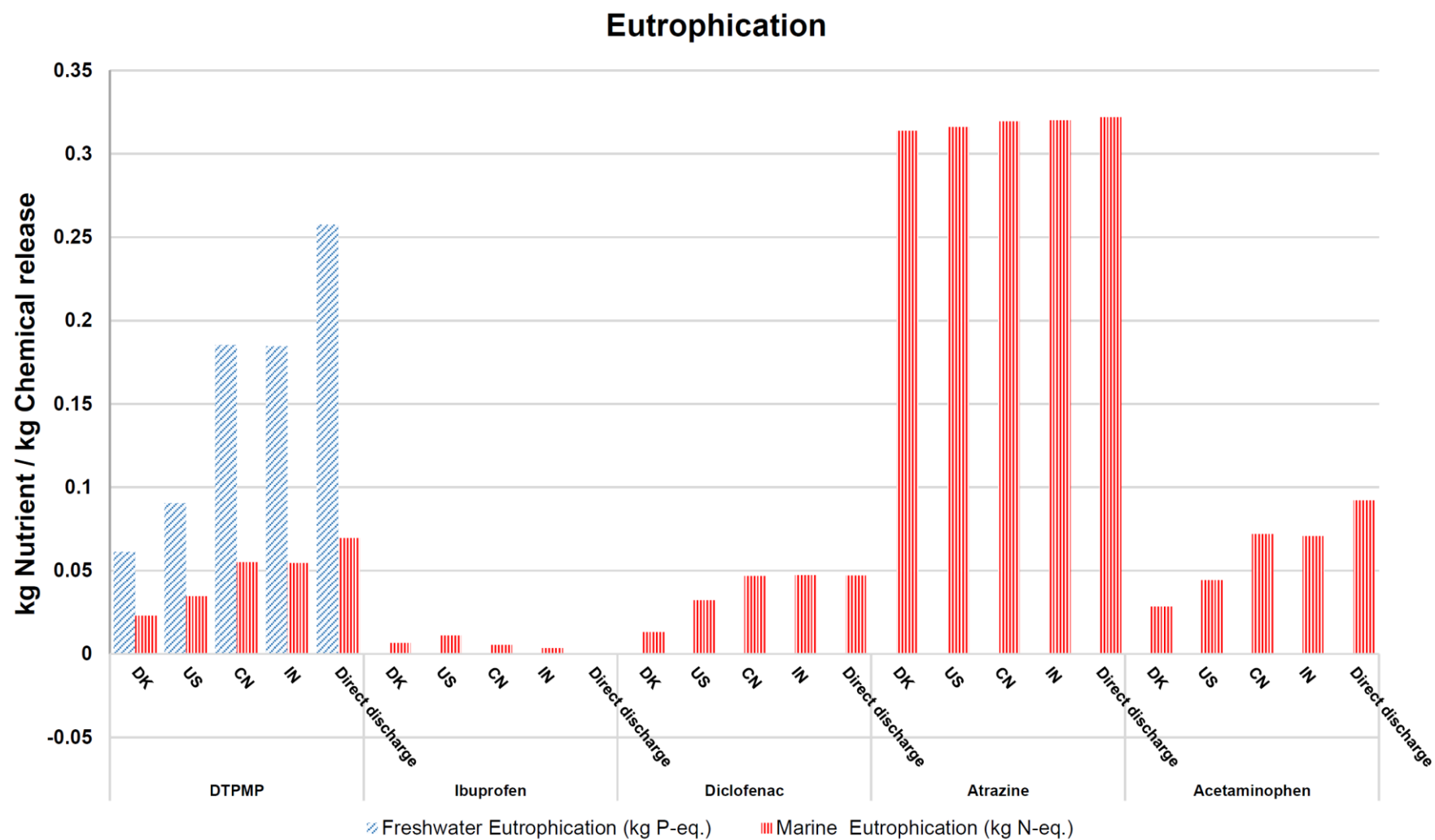


Figure 4: Impact assessment results for eutrophication

**Supplementary Information for**

**WW LCI v2: a second-generation life cycle inventory  
model for chemicals discharged to wastewater systems**

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Table S1: Parameters used in WW LCI 2.0

Parameters for degradation in the environment	Value	Definition/comments/source
$MCF_w$	0.1	Fraction of water compartments in the environment under anaerobic conditions. Muñoz et al. (2013)
$MCF_{sed}$	0.5	Fraction of sediments compartments in the environment under anaerobic conditions. Muñoz et al. (2013)
$f_{ox}$	0.5	Fraction of methane formed in sediments compartments that is oxidized to carbon dioxide. Muñoz et al. (2013)
$f_{CH_4}$	0.6	Fraction of carbon converted to methane when degraded under anaerobic conditions (Muñoz et al. (2013)
$EF_a$	0.01	N <sub>2</sub> O emission factor for the air compartment: fraction of N in the air compartment that is converted to N-N <sub>2</sub> O through re-deposition in soil and water (kg N-N <sub>2</sub> O / kg N). Muñoz et al. (2013)
$EF_s$	0.01	N <sub>2</sub> O emission factor for the soil compartment: fraction of N in soil that is converted to N-N <sub>2</sub> O (kg N-N <sub>2</sub> O / kg N). Muñoz et al. (2013)
$Ef_w$	0.005	N <sub>2</sub> O emission factor for the water compartment: fraction of N in water that is converted to N-N <sub>2</sub> O (kg N-N <sub>2</sub> O / kg N). Muñoz et al. (2013)
$EF_{sed}$	0.005	N <sub>2</sub> O emission factor for the sediments compartment: fraction of N in sediments that is converted to N-N <sub>2</sub> O (kg N-N <sub>2</sub> O / kg N). Muñoz et al. (2013)
Parameters for WWTP	Value	Definition/comments/source
C assimilation in biomass	0.55	Fraction of carbon in substrate that is converted to biomass in carbonaceous organic matter degradation reaction. Jimenez-Gonzalez et al. (2001)
C oxidation	0.45	Equals (1 - C assimilation in biomass). Fraction of carbon in substrate that is converted to carbon dioxide in carbonaceous organic matter degradation reaction. Jimenez-Gonzalez et al. (2001)
Extent of nitrification (If N removal)	0.84	Fraction ammonia-N that is converted to nitrate in a plant applying N removal. Estimate based on Doka (2007) and Lauver and Baker (2000)
Extent of denitrification (If N removal)	0.876	Fraction nitrate-N that is converted to nitrogen gas in a plant applying N removal. Estimate based on Doka (2007) and Lauver and Baker (2000)
Extent of nitrification (If no N removal)	0	Fraction ammonia-N that is converted to nitrate in a plant without N removal.



		Assumed zero
Extent of denitrification (If no N removal)	0	Fraction nitrate-N that is converted to nitrogen gas in a plant without N removal. Assumed zero
N-N <sub>2</sub> O (kg emitted per kg N biodegraded)	0.005	Fraction of nitrogen input converted to N-N <sub>2</sub> O. Average from Dalemo (1997) (0.15%) and Doka (2007) (0.68%)
Degradation ratio in sludge digester	0.6	Fraction of volatile solids converted to biogas in anaerobic digester. Assumes 20 days solids retention time (Appels et al. 2008)
C conversion to methane in sludge digester	0.5	Fraction of carbon in anaerobic digester converted to methane. Dalemo et al. (1997)
Methane higher calorific value (MJ/kg)	55.53	Engineering toolbox 2015
Methane emission factor in combustion (kg/MJ)	0.0001	Emission factor for methane in combustion of biogas from anaerobic digestion. Dalemo (1997)
Electricity (kWh/kg O <sub>2</sub> )	1.1	Electricity consumption factor for oxygen supplied to biodegradation reactions in WWTP. Jimenez-Gonzalez et al. (2001)
Electricity (kWh/kg dry solids to digestion)	0.448	Electricity consumption factor for sludge treatment in WWTP. Doka (2007): 0.28 kWh/m <sup>3</sup> *20% for sludge/0.125 kg solids/m <sup>3</sup> = 0.448 kWh/kg solids
Electricity conversion efficiency of biogas	0.35	Fraction of energy from combustion of biogas converted to electricity in a combined heat and power plant in a WWTP. Hopkowitz (2000)
Heat conversion biogas	0.55	Fraction of energy from combustion of biogas converted to heat in a combined heat and power plant in a WWTP. Hopkowitz (2000)
% electricity miscellaneous	0.1	Fraction of electricity demand in WWTP used for general purposes (Doka 2007)
% heat miscellaneous	0.1	Fraction of heat demand in WWTP used for general purposes (Doka 2007)
Electricity consumption by plant (kWh/m <sup>3</sup> )	0.28	Overall electricity demand of a WWTP (Doka 2007)
Heat demand WWTP (MJ/m <sup>3</sup> )	0.99	Overall heat demand of a WWTP (Doka 2007)
Heat demand by sludge processes (MJ/kg dm raw sludge)	7.128	Based on Doka (2007): 0.99 MJ/m <sup>3</sup> , 125 g raw sludge/m <sup>3</sup> , 90% of energy used for sludge and 10% for miscellaneous
mol weight of biomass including P	115.294	Molecular weight of biomass sludge, based on empirical formula including phosphorus (C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub> P <sub>0.031</sub> ), Droste et al. (1997)
mol weight of biomass excluding P	113	Molecular weight of biomass sludge, based on empirical formula excluding phosphorus (C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub> )
Chemical P removal level (%)	80%	Etienne et al. <a href="http://www.ncbi.nlm.nih.gov/pubmed/11804358">http://www.ncbi.nlm.nih.gov/pubmed/11804358</a>

FeCl <sub>3</sub> consumption (kg/kg P removed)	7.86	Iron chloride consumption factor in chemical phosphorus removal, assuming 50% excess Fe. Paul et al. (2001)
Chemical sludge formation (FePO <sub>4</sub> +Fe(OH) <sub>3</sub> ) (kg/kg P removed)	6.60	Chemical sludge formation factor in chemical phosphorus removal, assuming 50% excess Fe. Paul et al. (2001)
degradable S in digester that scapes in biogas (%)	22%	Percentage of sulfur in sludge that is partitioned to biogas in the anaerobic digester (Doka 2007)
Solids in thickened sludge entering digestion (%)	3%	Gravity thickening average for primary+secondary sludge (Daigger 1998, p. 164)
WWTP infrastructure (unit/m <sup>3</sup> )	6.06E-10	Amount of WWTP infrastructure attributed to 1 m <sup>3</sup> wastewater, according to Ecoinvent 3, average sewage, plant capacity 4.7E10L/year
Sewer infrastructure (km/m <sup>3</sup> )	1.24E-07	Amount of sewer infrastructure attributed to 1 m <sup>3</sup> wastewater, according to Ecoinvent 3, average sewage, plant capacity 4.7E10L/year
N speciation in biogas flare (%), N <sub>2</sub>	91.8%	Percentage of N in biogas flare that occurs as nitrogen gas (Doka, 2007, table 4.21)
N speciation in biogas flare (%), NO <sub>x</sub> (as NO <sub>2</sub> )	5.6%	Percentage of N in biogas flare that occurs as nitrogen oxides-N (Doka, 2007, table 4.21)
N speciation in biogas flare (%), N <sub>2</sub> O	0.9%	Percentage of N in biogas combustion that occurs as dinitrogen monoxide-N (Doka, 2007, table 4.21)
N speciation in biogas flare (%), NH <sub>3</sub>	1.7%	Percentage of N in biogas combustion that occurs as ammonia-N (Doka, 2007, table 4.21)
Dry matter content of biomass cells (%)	30.0%	Dry mass in activated sludge cells, expressed as percentage. Refers to bacteria (Nature 2014)
Solids in dewatered sludge (%)	30.0%	Dry mass in average dewatered sludge, expressed as percentage. Assumption.
<b>Parameters for sludge disposal</b>	<b>Value</b>	<b>Definition/comments/source</b>
Transport distance to landfarming (km)	20	Assumption
Transport distance to landfill (km)	20	Assumption
Transport distance to incinerator (km)	20	Assumption
Transport distance to composting plant (km)	20	Assumption
Compost plant infrastructure (units/kg biowaste wet weight)	4E-09	Amount of composting plant infrastructure attributed to 1 kg biowaste sent to composting, in wet weight. Data from ecoinvent dataset 'Biowaste {CH}' treatment of, composting'
Electricity use in composting (kWh/kg sludge)	0.00106	3.8 MJ/tonne sludge in wet weight (Poulsen and Hansen 2003, table 2).

Diesel use in composting (MJ/kg sludge)	0.0765	1.7 kg diesel oil per tonne sludge in wet weight (Poulsen and Hansen 2003, table 2). Calorific value of diesel is 45 MJ/kg according to the same source.
Extent of degradation for degradable chemicals (%)	0.65	Average for 5 different degradable materials (lignin, cellulose, carbohydrate, fat, protein) from Sonesson (1996, table 4).
Methane emission during composting (kg CH <sub>4</sub> /kg degradable dry matter)	0.01	IPCC (2006b)
Carbon content in average degradable dry matter in compost plants (kg C/kg dry matter)	0.435	Average from typical materials sent to composting: food and garden waste. Data from IPCC (2006b)
N loss as N <sub>2</sub> O (%)	0.02	Sonesson (1996)
N loss as N <sub>2</sub> (%)	0.02	Sonesson (1996)
N loss as NH <sub>3</sub> (%)	0.82	Based on Sonesson (1996) that gives 96% of N escaping as NH <sub>3</sub> . We assume 85% of this stays as NH <sub>3</sub> , while the 15% remaining is converted to NO <sub>x</sub> . This is based on a fixed ratio between NH <sub>3</sub> -N and NO <sub>x</sub> -N at 0.85 : 0.15 (based on FAO and IFA 2001, table 10&13)
N loss as NO <sub>x</sub> (%)	0.14	Based on Sonesson (1996) that gives 96% of N escaping as NH <sub>3</sub> . We assume 85% of this stays as NH <sub>3</sub> , while the 15% remaining is converted to NO <sub>x</sub> . This is based on a fixed ratio between NH <sub>3</sub> -N and NO <sub>x</sub> -N at 0.85 : 0.15 (based on FAO and IFA 2001, table 10&13)
Moisture content in compost (%)	0.5	Sonesson (1996)
Mass reduction during composting in wet weight (%)	0.57	Poulsen and Hansen (2003)
Dry matter content in sludge sent for composting (%)	0.28	Poulsen and Hansen (2003)
Frac_GASF	0.1	kg N volatilised / kg of N applied. Fraction of synthetic fertiliser N that volatilises as NH <sub>3</sub> and NO <sub>x</sub> , kg N volatilised (kg of N applied) <sup>-1</sup> (IPCC 2006, Table 11.3)
Frac_GASM	0.2	kg N volatilised / kg of N applied or deposited. Fraction of applied organic N fertiliser materials (FON) and of urine and dung N deposited by grazing animals (F_PRP) that volatilises as NH <sub>3</sub> and NO <sub>x</sub> , kg N volatilised (kg of N applied or deposited) <sup>-1</sup> (IPCC, 2006, Table 11.3)
Frac_LEACH	0.3	kg N / kg of N additions. Fraction of all N added to/mineralised in managed soils in regions where leaching/runoff occurs that is lost through leaching and runoff, kg N (kg of N additions) <sup>-1</sup> (IPCC 2006)
EF1	0.01	kg N <sub>2</sub> O–N / kg N input. Emission factor for N <sub>2</sub> O emissions from N inputs (IPCC 2006, Table 11.1)



EF4	0.01	kg N-N <sub>2</sub> O/ (kg NH <sub>3</sub> -N + NO <sub>x</sub> -N). Emission factor for N <sub>2</sub> O emissions from atmospheric deposition of N on soils and water surfaces, [kg N-N <sub>2</sub> O (kg NH <sub>3</sub> -N + NO <sub>x</sub> -N volatilised)-1] (IPCC, 2006, Table 11.3)
EF5	0.0075	kg N <sub>2</sub> O-N/ kg N leached and runoff. Emission factor for N <sub>2</sub> O emissions from N leaching and runoff, kg N <sub>2</sub> O-N (kg N leached and runoff)-1 (IPCC, 2006, Table 11.3)
NO <sub>x</sub> -N	0.15	kg NO <sub>x</sub> / yr. Fixed ratio between NH <sub>3</sub> -N and NO <sub>x</sub> -N at 0.85 : 0.15 (based on FAO and IFA 2001, table 10&13)
NH <sub>3</sub> -N	0.85	kg NH <sub>3</sub> -N ha <sup>-1</sup> yr <sup>-1</sup> . Fixed ratio between NH <sub>3</sub> -N and NO <sub>x</sub> -N at 0.85 : 0.15 (based on FAO and IFA 2001, table 10&13)
Replacement ratio of mineral N	0.4	kg mineral N avoided per kg N applied in sludge (Boldrin et al. 2009)
Replacement ratio of mineral P	0.95	kg mineral P avoided per kg P applied in sludge (Boldrin et al. 2009)
<b>Parameters for Primary treatment</b>	<b>Value</b>	<b>Definition/comments/source</b>
Fsludge in Primary Treatment compared to full WWTP with secondary treatment ( $r_{deg.pt}$ )	30%	Assumption based on Metcalf et al. (2007)
Fdeg in Primary Treatment compared to full WWTP with secondary treatment ( $r_{sludge.pt}$ )	30%	Assumption based on Metcalf et al. (2007)
Fair in Primary Treatment compared to full WWTP with secondary treatment ( $r_{air.pt}$ )	0%	Assumption
Electricity (kWh/kg dry solids to digestion)	0.399	Estimated based on Stillwell et al. (2010)
Electricity consumption by plant (kWh/m <sup>3</sup> )	0.09	Estimated based on Stillwell et al. (2010)
WWTP infrastructure (unit/m <sup>3</sup> )	1.82E-10	Assumed 30% of WWTP infrastructure
<b>Parameters for Septic Tank</b>	<b>Value</b>	<b>Definition/comments/source</b>
Fsludge in Septic Tank compared to full WWTP with secondary treatment ( $r_{sludge.st}$ )	30%	Assumption based on UNEP/GPA (2004)
Fdeg in Septic Tank compared to full WWTP with secondary treatment ( $r_{deg.st}$ )	30%	Assumption based on UNEP/GPA (2004)
Fair in Septic Tank compared to full WWTP with secondary treatment ( $r_{air.st}$ )	0%	Assumption
Sludge Transport Distance (km)	50	Assumption
Use of PVC for septic tanks (kg/kg wastewater)	0.12	From Pizzol et al. (2015)

Use of polyethylene for septic tanks (kg/kg wastewater)	0.11	From Pizzol et al. (2015)
Use of injection moulding for septic tanks (kg/kg wastewater)	0.23	From Pizzol et al. (2015)
Excavation for septic tanks (m3/kg of wastewater)	0.05	From Pizzol et al. (2015)
Use of sand for septic tanks (kg/kg of wastewater)	17.5	From Pizzol et al. (2015)
Use of gravel for septic tanks (kg/kg of wastewater)	3.28	From Pizzol et al. (2015)
<b>Parameters for Tertiary Treatment</b>	<b>Value</b>	<b>Definition/comments/source</b>
pH of wastewater	6.50	Metcalf et al. (2007)
foc,sludge in Tertiary Treatment	0.35	The fraction of organic carbon in sludge [-]
Density of sludge in Tertiary Treatment (g/L)	721	Andersen et al. (2004)
Transformation, from unknown in tertiary treatment (m2/m3 of wastewater)	2.74E-05	Derived from Muñoz et al. (2010)
Transformation, to industrial area, built-up, in tertiary treatment (m2/m3 of wastewater)	2.74E-05	Derived from Muñoz et al. (2010)
Occupation, industrial area, built up, in tertiary treatment (m2y/m3 of wastewater)	6.85E-04	Derived from Muñoz et al. (2010)
Building for tertiary treatment (m2/m3 of wastewater)	2.74E-05	Derived from Muñoz et al. (2010)
Use of sand for sand filter (kg/m3 of wastewater)	0.016	Derived from Muñoz et al. (2010)
Sodium hydroxide for cleaning (kg/m3 of wastewater)	0.0075	Derived from Muñoz et al. (2010)
Electricity use for sand filter (kWh/m3 of wastewater)	0.024	Derived from Muñoz et al. (2010)

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Table S2: Physico-chemical properties of assessed chemicals

Name	CAS number	Type	Composition (no of atoms in a molecule)							Molecular weight (g/mol)	Kow	pKa	Biogenic carbon?	Neutral/Acid/Base	Vapour pressure 25 deg. C (Pa)	Solubility 25 deg (mg/L)	Melting point (deg. C)	Koc	Henry's Law Constant (Pa·m3/mol)
			C	H	O	N	S	P	Cl										
Diclofenac	15307-86-5	Organic	14	11	2	1			2	296.15	32359	4.11	no	A	8.2E-06	2.37	284	245	0.0010
Ibuprofen	15687-27-1	Organic	13	18	2					206.29	9332	4.53	no	A	0.0248	21	76	3400	0.24362
Atrazine	1912-24-9	Organic	8	14		5			1	215.69	407	1.22	no	B	3.9E-05	34.7	174	173.78	0.00024
DTPMP	15827-60-8	Inorganic	9	28	15	3		5		573.00	0.00		no	-	1.7E-10	500000	90		7.4E-13
Acetaminophen	103-90-2	Organic	8	9	2	1				151.17	2.88	9.48	no	A	0.00026	14000	168	21	2.8E-06

Table S3: Fate of chemicals in Wastewater Treatment Plant and in environment

Name	CAS number	Type	Fate in WWTP (%)					Fate in environment (%)											
			Estimated from Simpletreat Model				Assessed using EPI Suite	Estimated using USESLCA model											
			Fair	Fdeg	Fsludge	Anaerobic deg?		If emitted to water				If emitted to soil				If emitted to air			
								Dega	Degw	Degsed	Degs	Dega	Degw	Degsed	Degs	Dega	Degw	Degsed	Degs
Diclofenac	15307-86-5	Organic		0.00%	0.94%		no	0.00%	99.51%	0.38%	0.00%	0.15%	4.21%	0.02%	95.62%	26.95%	35.41%	0.02%	37.60%
Ibuprofen	15687-27-1	Organic		0.00%	72.07%		no	0.04%	99.40%	0.49%	0.01%	0.08%	2.27%	0.01%	97.64%	55.43%	26.56%	0.01%	17.97%
Atrazine	1912-24-9	Organic		0.00%	1.13%		no	0.01%	98.83%	0.77%	0.02%	0.07%	4.86%	0.04%	95.02%	26.70%	38.00%	0.06%	35.18%
DTPMP	15827-60-8	Inorganic		0.00%	0.00%		no	0.00%	53.11%	42.13%	0.00%	0.09%	0.44%	0.35%	99.08%	4.45%	41.19%	3.79%	50.41%
Acetaminophen	103-90-2	Organic		0.00%	86.85%		no	0.00%	99.06%	0.84%	0.00%	0.06%	2.46%	0.02%	97.46%	4.96%	42.68%	0.04%	52.31%

Table S4: Key foreground inventory flows for the chemicals in four country scenarios

Denmark						USA					China					India				
Exchanges	Diclofe nac	Ibuprof en,	Atrazi ne,	DTPM PA	Acetamino phen	Diclofe nac	Ibuprof en,	Atrazi ne,	DTPM PA	Acetamino phen	Diclofe nac	Ibuprof en,	Atrazi ne,	DTPM PA	Acetamino phen	Diclofe nac	Ibuprof en,	Atrazi ne,	DTPM PA	Acetamino phen
Electricity (kWh/kg)																				
WWTP	0.0020	0.4860	0.0078	0.0105	0.1849	0.0016	0.3868	0.0062	0.0090	0.1477	0.0008	0.1841	0.0029	0.0038	0.0699	0.0005	0.1210	0.0019	0.0038	0.0473
Sludge disposal	-0.2053	-0.0968	-0.0047	-0.1147	-0.0171	-0.0358	0.0784	-0.0004	-0.0353	0.1006	0.0001	0.0255	0.0002	-0.0039	0.0261	0.0000	0.0000	0.0000	0.0000	0.0000
Total	-0.2033	0.3892	0.0031	-0.1042	0.1678	-0.0341	0.4652	0.0058	-0.0263	0.2483	0.0009	0.2096	0.0031	-0.0001	0.0960	0.0005	0.1210	0.0019	0.0038	0.0473
Heat (MJ/kg)																				
WWTP	-0.0015	-0.1843	-0.0018	0.1642	-0.1883	-0.0122	-1.3928	-0.0144	0.1360	-1.4220	-0.0103	-1.1611	-0.0122	0.0600	-1.1852	-0.0060	-0.7141	-0.0070	0.0602	-0.7294
Sludge disposal	-1.3564	-0.6246	-0.0062	-0.6423	-0.0414	-0.2422	0.2206	-0.0005	-0.2082	0.3752	-0.0001	0.0560	0.0001	-0.0247	0.0578	0.0000	0.0000	0.0000	0.0000	0.0000
Total	-1.3580	-0.8090	-0.0080	-0.4781	-0.2297	-0.2544	-1.1722	-0.0149	-0.0722	-1.0468	-0.0105	-1.1051	-0.0121	0.0354	-1.1274	-0.0060	-0.7141	-0.0070	0.0602	-0.7294
Chemicals (kg pure chemical/kg)																				
Methanol	0.0000	0.0000	0.0046	0.0000	0.0148	0.0000	0.0000	0.0037	0.0000	0.0118	0.0000	0.0000	0.0018	0.0000	0.0056	0.0000	0.0000	0.0011	0.0000	0.0036
Iron chloride	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Sludge to disposal (kg dry mass/kg) <sup>a</sup>																				
WWTP	0.8341	0.4993	0.0244	0.7727	0.2718	0.4085	0.3439	0.0198	0.6521	0.2330	0.0053	0.0987	0.0081	0.2805	0.0979	0.0054	0.0990	0.0081	0.2814	0.0979
Fertilizers (kg nutrient/kg)																				
Nitrogen fertiliser, as N	-0.0089	-0.0054	-0.0016	-0.0128	-0.0055	-0.0041	-0.0040	-0.0012	-0.0100	-0.0041	-0.0001	-0.0020	-0.0005	-0.0046	-0.0020	-0.0001	-0.0037	-0.0010	-0.0083	-0.0038
Phosphate fertiliser, as P <sub>2</sub> O <sub>5</sub>	0.0000	0.0000	0.0000	-0.2560	0.0000	0.0000	0.0000	0.0000	-0.2007	0.0000	0.0000	0.0000	0.0000	-0.0928	0.0000	0.0000	0.0000	0.0000	-0.1656	0.0000
CO <sub>2</sub> emissions and storage (kg CO <sub>2</sub> /kg)																				
WWTP	0.0136	1.4004	0.0190	0.0000	1.4366	0.0113	1.1631	0.0156	0.0000	1.1925	0.0050	0.5138	0.0071	0.0000	0.5273	0.0046	0.4767	0.0059	0.0000	0.4872
Sludge disposal	0.7531	0.6843	0.0197	0.2313	0.4122	0.1361	0.2910	0.0072	0.0713	0.2449	0.0012	0.0886	0.0015	0.0079	0.0900	0.0014	0.1455	0.0016	0.0000	0.1481
Deg. in environment	1.2833	0.6521	1.4969	0.4249	0.4572	1.5852	1.0282	1.5007	0.4262	0.7263	1.9416	1.9794	1.5156	0.5036	1.5560	1.9456	1.9816	1.5205	0.5885	1.5547
Storage, long-term	0.0004	0.0002	0.0057	0.0076	0.0005	0.2029	0.1115	0.0128	0.1188	0.0362	0.0052	0.0215	0.0094	0.0812	0.0199	0.0023	0.0012	0.0058	0.0237	0.0017
Total	2.0505	2.7370	1.5413	0.6638	2.3066	1.9354	2.5938	1.5363	0.6163	2.1999	1.9531	2.6032	1.5335	0.5927	2.1932	1.9540	2.6050	1.5338	0.6122	2.1915
Nutrient emissions to water (kg substance/kg)																				
Ammonium	0.0000	0.0000	0.0007	0.0000	0.0022	0.0025	0.0000	0.0015	0.0062	0.0024	0.0000	0.0000	0.0006	0.0033	0.0007	0.0000	0.0000	0.0006	0.0000	0.0019
Nitrate	0.0341	0.0005	1.3813	0.0711	0.0892	0.1226	0.0128	1.3892	0.1080	0.1513	0.2066	0.0065	1.4102	0.2217	0.2986	0.2065	0.0000	1.4099	0.2211	0.2911
P-total	0.0000	0.0000	0.0000	0.0587	0.0000	0.0000	0.0000	0.0000	0.0897	0.0000	0.0000	0.0000	0.0000	0.1854	0.0000	0.0000	0.0000	0.0000	0.1851	0.0000
N <sub>2</sub> O emissions (kg N <sub>2</sub> O/kg)																				
WWTP	0.0000	0.0005	0.0000	0.0000	0.0006	0.0000	0.0004	0.0000	0.0000	0.0005	0.0000	0.0002	0.0000	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0002
Other	0.0004	0.0002	0.0025	0.0006	0.0004	0.0004	0.0002	0.0025	0.0005	0.0004	0.0004	0.0001	0.0025	0.0006	0.0006	0.0004	0.0001	0.0025	0.0007	0.0007
Total	0.0004	0.0007	0.0025	0.0006	0.0010	0.0004	0.0006	0.0025	0.0005	0.0009	0.0004	0.0003	0.0025	0.0006	0.0008	0.0004	0.0003	0.0026	0.0007	0.0008
Emission of assessed chemical (kg/kg)																				
To air	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
To water	0.1599	0.1098	0.9684	0.2273	0.2081	0.5865	0.3300	0.9741	0.3479	0.3319	0.9925	0.7587	0.9893	0.7195	0.7127	0.9925	0.7580	0.9892	0.7186	0.7118
To agricultural soil	0.4682	0.1324	0.0120	0.4350	0.0013	0.2125	0.0612	0.0090	0.3411	0.0009	0.0025	0.0019	0.0039	0.1576	0.0004	0.0044	0.0034	0.0070	0.2814	0.0007

Note: figures with negative signs are interpreted as credits. <sup>a</sup>Sludge is an intermediate flow between the WWTP and sludge disposal, thus it is not part of the final LCI. It is shown here for information only.